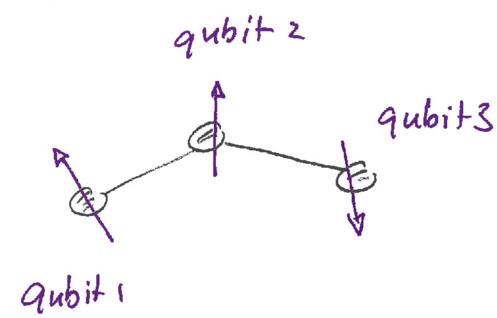
Phys 396 2018

Lecture 26

Constructing quantum gates.

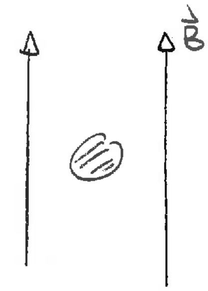
The way in which any quantum gates are realized physically depends on the particular physical system used to represent the qubits. We will illustrate this with the example of a "single molecule" NMR system. This consists of a molecule with several spin-½ nuclei. Provided that the nuclei are distinguishable, they each constitute a single qubit.



We need to consider how these qubits may evolve in the presence of external magnetic fields. Such evolution will eventually provide the gates that needed for quantum information processing.

Single qubit in a constant magnetic field

We begin by considering a single qubit in a constant magnetic field $\vec{B} = B_0 \hat{z}$. Then the energy operator for this, or Hamiltonian is



$$\hat{H} = \gamma \hbar \vec{B} \cdot \hat{\vec{\sigma}}$$

where $\gamma = \frac{ge}{2m}$ is a constant for the particular qubit.

Thus

$$\hat{H} = \gamma \hbar B_0 \hat{\sigma}_z$$

$$\hat{H} = \gamma \hbar B_0 \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

A standard result from quantum theory is that the eigenstates of the Hamiltonian are also the states that are associated with outcomes of energy measurements. Recall that an eigenstate satisfies

$$\hat{H}|\psi\rangle = E|\psi\rangle$$

where E is a constant. Here the eigenstates and associated energy values are

state	energy
$\|+\hat{z}\rangle$	$\gamma\hbar B_0$
$\|-\hat{z}\rangle$	$-\gamma\hbar B_0$

Thus the external magnetic field along $\hat{z}$ establishes a higher energy state and a lower energy state. It also determines the evolution of the state.

The key ingredient here is that the state vector satisfies:

$$\boxed{i\hbar \frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle}$$

- this is the Schrödinger equation

One can show that

$$\boxed{\begin{array}{l}\text{If } \hat{H} \text{ is independent of time then the solution to} \\ \quad i\hbar \dfrac{\partial}{\partial t} |\Psi(t)\rangle = \hat{H} |\Psi(t)\rangle \\ \text{is} \\ \quad |\Psi(t)\rangle = e^{-i\hat{H}t/\hbar} |\Psi_0\rangle \\ \text{where } |\Psi_0\rangle = |\Psi(t=0)\rangle \text{ is the initial state of the} \\ \text{system}\end{array}}$$

This enables us to start with the Hamiltonian and ultimately determine how the system evolves. Specifically it gives the evolution operator:

$$\hat{U}(t) = e^{-i\hat{H}t/\hbar}$$

1 Evolution of a single spin-1/2 system in a constant magnetic field

Consider a single spin-1/2 particle in a magnetic field $\mathbf{B} = B_0\hat{\mathbf{z}}$. Then

$$\hat{H} = \gamma\hbar B_0\hat{\sigma}_z.$$

a) Determine a matrix representing the evolution operator for this system.

b) Suppose that the qubit is initially in the state $|0\rangle = |+\hat{z}\rangle$. Determine the state of the system at any later time.

c) Suppose that the qubit is initially in the state $|1\rangle = |-\hat{z}\rangle$. Determine the state of the system at any later time.

d) Suppose that the qubit is initially in the state $(|0\rangle + |1\rangle)/\sqrt{2}$. Determine the state of the system at any later time. Describe the evolution of the state in terms of the Bloch sphere.

e) Describe how this could be used to construct the gate $\hat{\sigma}_z$.

f) Determine an expression for the angular frequency ω_0 of the evolution.

Answer: a) $\hat{U}(t) = e^{-i\hat{H}t/\hbar}$

$$= e^{-i\gamma B_0 t\,\hat{\sigma}_z}$$

Let $\gamma B_0 t = \theta$. Then this is

$$\hat{U} = e^{-i\theta\hat{\sigma}_z}$$

$$= \hat{I}\cos\theta - i\sigma_z\sin\theta = \begin{pmatrix} \cos\theta - i\sin\theta & 0 \\ 0 & \cos\theta + i\sin\theta \end{pmatrix}$$

$$= \begin{pmatrix} e^{-i\theta} & 0 \\ 0 & e^{i\theta} \end{pmatrix} \Rightarrow \hat{U} = \begin{pmatrix} e^{-i\gamma B_0 t} & 0 \\ 0 & e^{i\gamma B_0 t} \end{pmatrix}$$

b) $|0\rangle = |+\hat{z}\rangle \leftrightarrow \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

$$\hat{U}|0\rangle = \begin{pmatrix} e^{-i\gamma B_0 t} & 0 \\ 0 & e^{i\gamma B_0 t} \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = e^{-i\gamma B_0 t}\begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$= e^{-i\gamma B_0 t}|+\hat{z}\rangle \leftrightarrow |+\hat{z}\rangle$$

c) $|1\rangle \rightsquigarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix}$. By same reasoning

$$\hat{U}|1\rangle = e^{i\gamma B_0 t}|1\rangle \quad \text{and} \quad |1\rangle$$

d) Here $|\psi_0\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$

$$\Rightarrow \quad |\psi\rangle = \frac{1}{\sqrt{2}}e^{-i\gamma B_0 t}|0\rangle + \frac{1}{\sqrt{2}}e^{i\gamma B_0 t}|1\rangle$$

$$= \underbrace{e^{-i\gamma B_0 t}}_{\text{global phase.}} \frac{1}{\sqrt{2}}\left\{|0\rangle + e^{i 2\gamma B_0 t}|1\rangle\right\}$$

$$\text{and} \quad \frac{1}{\sqrt{2}}\left\{|0\rangle + e^{i2\gamma B_0 t}|1\rangle\right\}$$

corresponds to state with $\theta = \pi/2$ $\phi = 2\gamma B_0 t$

e) Choose θ s.t. $\hat{U} = \underbrace{-i}_{\text{global phase}} \sigma_z$ i.e. $\theta = \pi/2$. Then

Then $\hat{U} = \hat{\sigma}_z$

f) After time t Bloch sphere state has rotated by $2\gamma B_0 t$

$\Rightarrow \omega_0 = 2\gamma B_0$

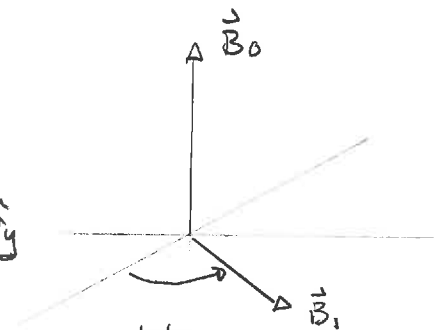
Single qubit in an oscillating magnetic field

Now suppose that the spin-½ particle is in a constant magnetic field along with one which is perpendicular + oscillates sinusoidally.

Here the constant field is $\vec{B}_0 = B_0 \hat{z}$ and the time varying field is

$$\vec{B}_1 = B_1 \cos(\omega t)\,\hat{x} + B_1 \sin(\omega t)\,\hat{y}$$

Then the Hamiltonian for the system is:



rotates

angular freq. ω

$$\hat{H} = \gamma\hbar B_0 \hat{\sigma}_z + \gamma\hbar B_1 \cos\omega t\, \hat{\sigma}_x + \gamma\hbar B_1 \sin\omega t\, \hat{\sigma}_y$$

So

$$\hat{H} = \frac{\hbar\omega_0}{2}\hat{\sigma}_z + \frac{\hbar\omega_1}{2}\left[\cos\omega t\,\hat{\sigma}_x + \sin\omega t\,\hat{\sigma}_y\right]$$

Again the state satisfies

$$i\hbar \frac{\partial}{\partial t}|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle$$

However, this time $\hat{H}$ depends on time and thus we cannot use

$$|\Psi(t)\rangle \cancel{=} e^{-i\hat{H}t/\hbar}|\Psi_0\rangle$$

There is a mathematical trick call working in the rotating reference frame This entails using

$$|\tilde{\Psi}(t)\rangle = e^{i\omega\hat{\sigma}_z t/2}|\Psi(t)\rangle \quad \Rightarrow \quad |\Psi(t)\rangle = e^{-i\omega\hat{\sigma}_z t/2}|\tilde{\Psi}(t)\rangle$$

This is called working in the rotating ref frame because if $|\Psi(t)\rangle = e^{-i\omega t\hat{\sigma}_z/2}|\Psi_0\rangle$ (i.e. $|\Psi(t)\rangle$ rotates about the z-axis with angular frequency ω) then $|\tilde{\Psi}(t)\rangle = |\Psi_0\rangle$ and this just appears to be constant.

Now

$$i\hbar\frac{\partial}{\partial t}|\tilde{\Psi}(t)\rangle = i\hbar\frac{i\omega\sigma_z}{2}\underbrace{e^{i\omega\hat{\sigma}_z t/2}|\Psi(t)\rangle}_{|\tilde{\Psi}(t)\rangle} + e^{i\omega\sigma_z t/2}\underbrace{i\hbar\frac{\partial|\Psi\rangle}{\partial t}}_{\hat{H}|\Psi\rangle}$$

$$= -\frac{\hbar\omega}{2}\hat{\sigma}_z|\tilde{\Psi}(t)\rangle + e^{i\omega\hat{\sigma}_z t/2}\left[\frac{\hbar\omega_0}{2}\hat{\sigma}_z + \frac{\hbar\omega_1}{2}(\cos\omega t\,\hat{\sigma}_x + \sin\omega t\,\hat{\sigma}_y)\right]|\Psi\rangle.$$

$$= -\frac{\hbar\omega}{2}\hat{\sigma}_z|\tilde{\Psi}(t)\rangle + \frac{\hbar\omega_0}{2}e^{i\omega\hat{\sigma}_z t/2}\hat{\sigma}_z e^{-i\omega\hat{\sigma}_z t/2}|\tilde{\Psi}(t)\rangle$$

$$+\frac{\hbar\omega_1}{2}\left[e^{i\omega\hat{\sigma}_z t/2}\cos\omega t\,\hat{\sigma}_x e^{-i\omega\hat{\sigma}_z t/2} + e^{i\omega\hat{\sigma}_z t/2}\sin\omega t\,\hat{\sigma}_y e^{-i\omega\hat{\sigma}_z t/2}\right]|\tilde{\Psi}(t)\rangle$$

Now mathematics gives:

$$e^{i\omega t\hat{\sigma}_z/2}\,\hat{\sigma}_z\,e^{-i\omega t\hat{\sigma}_z/2} = \hat{\sigma}_z$$

$$e^{i\omega t\hat{\sigma}_z/2}\,\hat{\sigma}_x\,e^{-i\omega t\hat{\sigma}_z/2} = \cos\omega t\,\hat{\sigma}_x - \sin\omega t\,\hat{\sigma}_y$$

$$e^{i\omega t\hat{\sigma}_z/2}\,\hat{\sigma}_y\,e^{-i\omega t\hat{\sigma}_z/2} = \sin\omega t\,\hat{\sigma}_x + \cos\omega t\,\hat{\sigma}_y$$

Thus:

$$i\hbar\frac{\partial}{\partial t}|\tilde{\Psi}(t)\rangle = \Big[-\frac{\hbar\omega}{2}\hat{\sigma}_z + \frac{\hbar\omega_0}{2}\hat{\sigma}_z + \frac{\hbar\omega_1}{2}\hat{\sigma}_x(\cos^2\omega t + \sin^2\omega t)$$
$$+\frac{\hbar\omega_1}{2}\hat{\sigma}_y(-\cos\omega t\,\sin\omega t + \sin\omega t\,\cos\omega t)\Big]|\tilde{\Psi}(t)\rangle$$

$$= \Big[\frac{\hbar}{2}(\omega_0-\omega)\hat{\sigma}_z + \frac{\hbar\omega_1}{2}\hat{\sigma}_x\Big]|\tilde{\Psi}(t)\rangle$$

Thus

$$i\hbar\frac{\partial}{\partial t}|\tilde{\Psi}(t)\rangle = \hat{H}_{rot}|\tilde{\Psi}(t)\rangle$$

where

$$\hat{H}_{rot} = \frac{\hbar}{2}(\omega_0-\omega)\hat{\sigma}_z + \frac{\hbar\omega_1}{2}\hat{\sigma}_x$$

is a time-independent rotating frame Hamiltonian. It then follows that

$$|\tilde{\Psi}(t)\rangle = e^{-i\hat{H}_{rot}t/\hbar}|\tilde{\Psi}(0)\rangle$$

Finally since $|\psi(t)\rangle = e^{-i\omega\sigma_z t/2}|\psi\rangle$ we get

$$\boxed{|\psi(t)\rangle = e^{-i\omega\hat{\sigma}_z t/2}\, e^{-i\hat{H}_{rot} t/\hbar}\,|\psi(0)\rangle.}$$

Exercise: How must ω be chosen in relation to ω_0 to create a rotation about $\hat{x}$?

Answer: We need $\hat{H}_{rot} = \text{const} \times \hat{\sigma}_x$ Thus choose $\omega = \omega_0$ Then

$$|\psi(t)\rangle = e^{-i\omega_0\sigma_z t/2}\, e^{-i\,\omega_1\hat{\sigma}_x t/2}\,|\psi(0)\rangle$$

If we subsequently let the system evolve under B_0 for a period of time t' then the state of the system would be

$$|\psi(t)\rangle = e^{-i\omega_0\sigma_z(t+t')/2}\, e^{-i\hbar\omega_1\sigma_x t/2}\,|\psi(0)\rangle$$

We can always choose t' s.t. $\omega_0(t+t')/2 = 2\pi$. Then we get

$$|\psi(t)\rangle = e^{-i\hbar\omega_1\sigma_x t/2}\,|\psi(0)\rangle.$$

To map $|0\rangle \to |1\rangle$ we need

$$e^{-i\omega_1 \hat{\sigma}_x t/2} = \hat{\sigma}_x$$

$$\parallel$$

$$\cos(\omega_1 t/2)\,\hat{I} - i\hat{\sigma}_x \sin(\omega_1 t/2) = \hat{\sigma}_x$$

So $\omega_1 t/2 = \pi \Rightarrow t = \frac{2\pi}{\omega_1}$ "π-pulse"

To map $|0\rangle \to (|0\rangle - i|1\rangle)\frac{1}{\sqrt{2}}$ we need

$\sin\left(\frac{\omega_1 t}{2}\right) = \frac{1}{\sqrt{2}} \Rightarrow t = \frac{2\pi}{2\omega_1}$ "$\pi/2$-pulse"

2 Single qubit rotation about the x axis

Consider a single spin-1/2 particle in the situation described in the lecture.

a) How must ω be chosen in relation to ω_0 in order to create a rotation about the x axis.

b) How must the time of evolution be chosen in relation to ω_1 so that the evolution maps $|0\rangle \to |1\rangle$?

c) How must the time of evolution be chosen in relation to ω_1 so that the evolution maps

$$|0\rangle \to \frac{1}{\sqrt{2}}\left(|0\rangle - i\,|1\rangle\right)?$$